PAPER REFERENCE:

KINETIC MONTE CARLO SIMULATIONS: AN ACCURATE BRIDGE BETWEEN AB INITIO CALCULATIONS AND STANDARD PROCESS EXPERIMENTAL DATA

M. Jaraiz^{*}, E. Rubio, P. Castrillo, L. Pelaz, L. Bailon, J. Barbolla G. H. Gilmer¹, and C. S. Rafferty¹

E.T.S.I. Telecomunicacion, 47011 Valladolid, Spain ¹Bell Laboratories, Lucent Technologies, Murray Hill, New Jersey 07974

Abstract

Kinetic Monte Carlo (KMC) atomistic process simulations mimic the jumps and interactions of individual atoms, based on jump rates derived from ab initio calculations or experiments. By only following 'defect' atoms (unlike molecular dynamics), KMC can simulate the typical long annealing times (seconds to hours) used in materials processing. Thus, it provides a detailed and accurate link between parameters obtained from ab initio calculations and experiments performed under typical processing conditions. We describe the simulation scheme and discuss some of the unique features of this simulation technique with the help of results obtained with it.

Keywords

Monte Carlo, ab initio, process simulation.

Introduction

The level of refinement reached by today's materials processing technologies is calling for new modeling and simulation schemes, capable of handling the rich variety of interaction mechanisms that govern such complex processes at the atomic level. These modeling needs are a subject of increasing concern for the semiconductor industry as manifested in the 1997 SIA Roadmap which identifies atomistic process modeling among the difficult challenges below 100 nm: "Continuum physics models are no longer sufficient below 100 nm. Tools are needed for the physical and

* Corresponding Author:

Tel: +34 983 423677, Fax: +34 983 423675, Email: mjaraiz@ele.uva.es

chemical processes at an atomic level" [1]. We describe here a simulation scheme for diffusion and interaction of point and extended defects based on the kinetic Monte Carlo technique, which has, over the last few years, proved to be extremely powerful as a direct bridge between first principles calculations and standard materials processing data. For the case of polycrystalline materials, a lattice KMC method is also presented together with application examples.

The Kinetic Monte Carlo Approach

Molecular dynamics (MD) is the most accurate atomistic simulation technique. However, due to the fact that it simulates all the lattice atoms and, most importantly, that it uses an almost constant time step on the order of femtoseconds (10^{-15} s) , it cannot simulate the timescales involved in typical technological processing steps (seconds to hours). The kinetic Monte Carlo method, on the contrary, is an event-driven technique, i.e., simulates events at random with probabilities according to the corresponding event rates. In this way it self-adjusts the timestep as the simulation proceeds, depending on the fastest event present at that time. Figure 1 illustrates the concept behind the KMC approach: the figure shows a high resolution TEM view (from Ref. [2]) of a silicon sample with a {311} extended defect embedded in the silicon atomic rows. In MD, all of the lattice and defect atoms are simulated. In KMC, only the atoms belonging to point or extended defects are simulated (represented as circles on the TEM view). In the sample shown in Figure 1 one would see all the lattice atoms vibrating (with a period of about 10^{-13} s) and, from time to time (e.g. 10^{-9} s), one of the isolated point defects would jump to a neighboring position and can be captured by the extended defect. At even longer time intervals (e.g. 10^{-3} s) a point defect would be emitted from the extended defect. Since KMC only simulates the defect atoms, it starts out with timesteps on the order of 10⁻⁹ s. In addition, the fast moving point defects disappear very quickly, leaving only the extended defect and allowing the timestep to automatically be raised to 10^{-3} s. For example, the interstitial jump rate $(J_{rate,I})$ is given by

$$J_{\text{rate,I}} = 6 \times D_0 \times \exp(-E_{\text{mig,I}}/kT) / \lambda^2$$

where D_0 is the diffusivity prefactor, $E_{mig,I}$ is the interstitial migration energy and λ is the jump distance. Figure 2 represents the total energy of a system consisting of a boron and silicon interstitial atoms, as the system goes through different configurations. The intermediate configuration corresponds to a BI pair which is assumed to be immobile, whereas B_i stands for a mobile interstitial boron. The activation energy for the emission of an I from the BI pair is:

$$E_{act,I} = E_{bind,I} + E_{mig,I}$$

where $E_{bind,I}$ is the binding energy of the interstitial to the boron. These energies, obtained from ab initio calculations [3] or estimated by fitting experimental data, are then used in the KMC simulator to determine each event rate and decide which event to perform next. In addition to point defects, a full KMC simulator should implement models for a variety of defect types like surfaces, clusters and agglomerates (e.g. B_mI_n). A more detailed description of the DADOS kinetic Monte Carlo simulator can be found in Ref. [4].

The computing resources currently available in workstations and PC's has effectively enabled the development of KMC-based technology process simulators, that have taken the simulation of

standard technologic processes to an unprecedented level of microscopic detail. Besides this, due to the KMC simulation methodology, it is extremely simple to implement and test new mechanisms. It can also handle up to thousands of different event rates (equivalent to the same number of rate equations) without any convergence-related problems (there are no equations to be solved in a KMC simulator).

Simulation examples

We have explored, over the last few years [4,5,6,7,8], the capabilities of the KMC approach as a technology process simulator, i.e., establishing a direct link between ab initio parameters and typical process experimental data, with the most encouraging results.

Figure 3 shows a plan view TEM (a) and the corresponding DADOS simulation (b). In addition to accurate quantitative predictions of the time evolution of the total number of interstitials in clusters, this type of simulator (unlike the continuum simulators) also describes the actual geometry of the defects which can play an important role in low energy implants, where their size is comparable to the distance to the surface.

Figure 4, from Ref. [6], shows the SIMS profiles in a sequence of anneal times at 800 °C along with the simulation results. Notice the excellent agreement between the model and the experiment over the entire run. The predicted electrically inactive or clustered boron also agrees with spreading resistance profilometry data (not plotted in the figure).

Lattice Kinetic Monte Carlo

The KMC simulator described above can be used with homogeneous (e.g. monocrystalline or amorphous) materials. For polycrystalline materials, however, the presence of grain boundaries requires a modified approach. The description of a lattice KMC code which simulates polycrystalline thin film deposition and annealing by modeling individual grains with arbitrary orientations and shapes and their interactions, can be found in [9]. Effects such as grain nucleation, columnar growth, faceting and texture appear in the course of the simulations.

The simulation scheme for each monocrystal can be seen in Ref. [10]. The basic idea is to define a 3D grid with the structure of the crystal lattice. Atoms are attached to these sites as they are being deposited. In addition, atoms can jump to empty neighboring sites, with a probability which is a function of the energy difference between the initial and final sites, and the substrate temperature. In the case of a polycrystal, however, the crucial point is how to deal with the grain boundaries. Atoms near them are allowed to jump to an adjacent microcrystal in order to minimize the interface energy. Near a grain boundary (Fig. 5) we can then consider that there are several possible sites (A2, B1) an atom can jump into, each belonging to a different crystal orientation. When atom A1 is going to jump to a grain boundary site (A2), it checks the energy of the nearest sites (B1) in the adjacent microcrystals and finally it is attached to the one with highest coordination (B1). When a new atom is deposited, if it lands next to a previously deposited atom then the newly deposited atom is attached to the microcrystal of that atom. On the other hand, if it lands on the substrate surface and there is no other atom in the neighborhood, a new microcrystal with a different orientation is

created. The new lattice tilt and rotation angles are chosen either randomly or based on the substrate topology.

Some of the parameters needed are the potential energy of a surface atom as a function of its coordination, i.e., of the number of neighboring atoms (Fig. 6, from Ref. [10]). The figure shows that there is only a small variation in energy between the different possible configurations for a given coordination. These energies were calculated based on the embedded atom method (EAM) potential for aluminum.

Simulation Examples

The main feature of this type of approach is again the fact that it can simulate time intervals comparable to real processing times, while using atomic scale parameters like the above mentioned potential energies which can be readily obtained from ab initio calculations. As an example [11] Figure 7 shows the microcrystalline structure resulting from the simulation of aluminum deposition for two different substrate wetting conditions, modeled as a weakening of the bonding to the substrate. Weaker bonding (Fig. 7b) allows for more surface diffusion on the substrate to occur. This, in turn, leads to a reduction of the number of nucleation sites and, in the end, to a smaller number of grains and to larger grain sizes, as compared to Fig. 7a.

Conclusions

Kinetic Monte Carlo methods, applied to materials processing simulation, allow the direct use of parameters obtained from first principles calculations, thus establishing a bridge that can be highly beneficial for both the computational materials science and the microelectronics industry communities. Whilst KMC provide only a simplified description of the rich ab initio scenario, it seems to be the best projection of such a scenario into the dimensions and timescales involved in materials processing. KMC simulation can be used by the first principles scientific community as a means to check parameters obtained from ab initio calculations versus experimental data from standard processing measurements. On the other hand, KMC can nowadays provide an effective method to simulate microelectronics processing, in some cases even at full device dimensions, with an unprecedented level of detail. Finally, both communities can benefit from this synergistic bridge to increase the flow of knowledge between both ends and integrate ab initio materials calculations into process simulation.

Figure captions

Figure 1. TEM view of a {311} defect in silicon (from Ref. [2]). Circles represent the defect atoms simulated by the KMC method.

Figure 2. Total energy of a boron atom and a silicon interstitial as the system goes through different configurations.

Figure 3. Plan view TEM micrograph (a) (from Ref. [2]) and DADOS simulation (b) of a 40 keV 5×10^{13} cm⁻² silicon implant exhibiting {311} defects (from Ref. [4]).

Figure 4. Experimental SIMS profiles (thin lines) and DADOS simulation profiles (thick lines) for a boron doped layer after a 40 keV 9×10^{13} cm⁻² silicon implant and anneal at 800 °C. Thick dashed lines are the simulated boron in clusters (from Ref. [6]).

Figure 5. Schematic of the approach followed in an implementation of a polycrystal KMC simulator. Atom A1, initially jumping to site A2, is finally attached to the neighboring site B1 (higher coordination site) to minimize the grain boundary energy.

Figure 6. Potential energies of aluminum surface atoms as a function of coordination number (from Ref. [10]), from calculations based on the embedded atom method (EAM).

Figure 7. Microcrystalline structure resulting from the simulation of aluminum deposition for two different substrate wetting conditions: (a) wetting substrate, (b) non-wetting substrate (Ref. [11]).







Figure 2



(a)



(b)



Figure 4



Figure 5



Figure 6



(a)



(b)

References

- [1] National Technology Roadmap for Semiconductors 1997, p. 188.
- [2] P. A. Stolk, H. J. Gossmann, D. J. Eaglesham, D. C. Jacobson, C. S. Rafferty, G. H. Gilmer, M. Jaraiz, J. M. Poate,
- H. S. Luftman, and T. E. Haynes, J. Appl. Phys. 6031 (1997) 81.
- [3] J. Zhu, T. D. de la Rubia, L. H. Yang, C. Mailhiot, and G. H. Gilmer, Phys. Rev. B 4741 (1996) 54.
- [4] M. Jaraiz, L. Pelaz, E. Rubio, J. Barbolla, G. H. Gilmer, D. J. Eaglesham, H. J. Gossmann, and J. M. Poate, Mater. Res. Soc. Symp. Proc. 43 (1998) **532**.
- [5] M. Jaraiz, G. H. Gilmer, T. D. de la Rubia, and J. M. Poate, Appl. Phys. Lett. 409 (1996) 68.
- [6] L. Pelaz, M. Jaraiz, G. H. Gilmer, H. J. Gossmann, C. S. Rafferty, D. J. Eaglesham and J. M. Poate, Appl. Phys. Lett. 2285 (1997) 70.
- [7] L. Pelaz, G. H. Gilmer, M. Jaraiz, S. B. Herner, H. J. Gossmann, D. J. Eaglesham, G. Hobler, C. S. Rafferty, and J. Barbolla, Appl. Phys. Lett. 1421 (1998) 73.
- [8] L. Pelaz, G. H. Gilmer, V. C. Venezia, H. J. Gossmann, M. Jaraiz, and J. Barbolla, Appl. Phys. Lett. 2017 (1999) 74.
- [9] J. E. Rubio, M. Jaraiz, L. A. Bailon, J. Barbolla, M. J. Lopez, and G. H. Gilmer, Mater. Res. Soc. Symp. Proc. 127 (1998) **514**.
- [10] H. Huang, G. H. Gilmer, and T. D. de la Rubia, Phys. Rev. B 3636 (1998) 84.
- [11] E. Rubio, M. Jaraiz, L. Bailon, J. Barbolla (unpublished).